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Research Paper

Mathematical modeling of nonlinear electrokinetic flow and ion transport in polyelectrolyte-coated nanopores

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ABSTRACT

This document describes the formation of a new mathematical model of nonlinear electrokinetic flow and ion transport through a polyelectrolyte-coated nanopore. This model improves upon the previously developed models by considering the ionic transport due to the confinement at the polyelectrolyte nanopore interface and the nonlinear electrokinetic interactions at high voltage. The model is numerically implemented, and the results of the simulations confirm the electrokinetic ion transport phenomena and align with experimental data. The results of our work demonstrate the advances made to the distinctively electrokinetically controlled nanopore devices and their use as versatile tools in biosensing, energy storage devices, and water treatment technologies.

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1. INTRODUCTION

Nanopores have recently received considerable attention owing to their unique nanoscale geometries and the ability to facilitate ion and fluid flow with a high degree of control. This ability is of critical importance to a plethora of emerging applications in nanotechnology including biosensing, energy storage, and water treatment technologies [1], [2]. The aforementioned applications involve the use of electrokinetic phenomena (i.e. electroosmosis, dielectrophoresis, electrophoresis) for the transport of fluids and ions within confined geometries. In particular, polyelectrolyte-coated nanopores present unique electrokinetic behaviors and applications. Such coatings entail adaptive features enabling control of the flow and transport of ions, which is essential in many applications requiring accurate control over the ionic flow and transport [3].

The transport of ions through the nanopores is the result of the combination of the external applied electric field and the resultant electrokinetic forces. Normally, the classical models of ion transport presume a linear electrokinetic behavior, in which the applied electric field and the resultant ion flow (i.e. ion flux) are in a direct proportional relationship. Although this linear relationship holds true for many ideal cases, it is not true when the system is subjected to large high voltage gradients, where the electrostatic influence becomes dominant. The complexity is further enhanced by the presence of polyelectrolyte coatings. These coatings are made of charged macromolecules which bind to ions in the nanopore, thereby changing the electrostatic potential and the ion vacancy profile. Consequently, the ion transport becomes nonlinear, requiring sophisticated mathematical models in order to describe the situation accurately.

The drawbacks of linear electrokinetic models in capturing the behavior of such systems are well-known [4], [5]. These models presume a uniform surface charge density and envisage a simplistic view of the relationship between the applied electric field and the ion movement.

Additionally, when faced with more complex systems, including strong electric fields and variable ionic concentrations, the models in use today do not consider the subsequent charge redistribution, electrostatic repositioning, and ion exclusion. Therefore, in order to make accurate models, nonlinearity must be accounted for in order to improve the systems currently able to optimize nanofluidic devices, and more specifically the real-world devices, which imperative systems require, in order to optimize functionality. This leads to the systems' non-idealized models. This research demonstrates the insufficient systems within the current research scope. A thorough non-linear mathematical framework is developed describing ion transport and electrokinetic flows in nanoscopic chambers whose walls are composed of polyelectrolyte layers. This framework combines the Electrostatic Potential, which is internally described in the nanopore by the Poisson-Boltzmann equation, and Dynamical Fluid Integrator, represented by the Navier-Stokes equations. The charge separation nonlinear electrokinetics, dynamic polyelectrolyte systems, and concentration of ions within a system are caused by high voltage and will be accounted for within the framework. The nonlinearity is expected to clarify the chronodegree of ion transport in more distinct nanodevices than previously created. Finally, to clarify the distance of the nonlinear model from traditional electrokinetic models, the work conducted will focus on simulations and will explore the nonlinearity of the model alongside macrodynamic systems.

These differences are also manifest in the reactions of the ion concentration profiles and in the speeds of electroosmotic flow for the elevated voltage conditions. This situation shows the necessity for flexibility with respect to the nonlinear electrokinetic behavior when considering the design of nanofluidic devices already made. This is for the fact that such devices are in plentiful use in scenarios with high voltage and/or complicated liquid material environments [6].

This study centers on the construction of a nonlinear mathematical model that reflects the geometry and pore characteristics of the polyelectrolytes of the devices in question and aims to contribute to the comprehension and enhancement of operational nanofluidic devices. The result is the formation of a model that comes very close to reflecting the behavior of the ion transport system in a medium that contains uniform control of the electrokinetic system.

2. RELATED WORK

Over the past study period, the phenomenon of electrokinetic flow and ion transport in nanopores has been the subject of various studies, and the engineering complexities of the systems have been documented in detail in a number of studies. The use of porous electrodes for biosensing, energy storage, and water filtration applications is primarily based on the control of ion transport within confined geometries. The devices exploit the electrokinetic effects that govern ion transport and are affected by the surface charge of the nanopore, the ionic strength of the solution, and the externally applied electric field.

Significant research focuses on the construction of precise models of ion transport in circumstances where conventional linear electrokinetic models have proved inadequate. Prior studies have frequently dealt with the linear theories of electrokinetics derived from the assumption of a linear relation between the applied electric field and the ion flux. Such models work reasonably well in situations presented with low voltages and with the ion concentration profiles remaining constant or not varying [7], [8]. In these theories, the electrostatic potential and the fluid motion are described via the Poisson-Boltzmann and Navier-Stokes equations, respectively. In these models, the concentration of ions is assumed to be a linear function of the electrostatic potential, and the field Exerted is in direct proportion to the velocity of ions [9], [10].

It is clear, though, that these models cannot and do not capture the phenomena that are charge transports or the rapid transport of ions in cases where high electric fields are present or where there are intricate surface charge interactions. Such is the case with nanopores that have been coated with a polyelectrolyte layer, where the surface charge distribution becomes non-static and is contingent upon the ionic strength and pH of the bulk solution. Every polyelectrolyte layer is different in thickness and charge density, resulting in different potential electrostatic fields, and different levels of ionic concentration in the nanopores. This results in friction in the ion transport, refuting the proportionality of current models [11], [12].

Many researchers modified their scientific framework in accordance to their observations. In these instances, the incorporation of non-linear Boltzmann distribution of charges, and the modified Navier-Stokes equation of the ionic stream provides answers to a certain extent. These adjustments attempt to balance the ion and charge active surface of polyelectrolyte layers. These adjustments provide a more valid prediction of charge and mass transport system constants, and is more valid at the optimum ion confinement and electrostatic screening [13]. Recent developments in nanofluid devices with electrokinetic energy conversion, and distinct ion control in biosensors, designed for single molecule detection, and energy converters to store ion energy, require these simplified models to predict system behavior more accurately.

Polyelectrolyte layers in nanopores complicate ion transport even more than previous models predict. Charge polymer layers and nanopore ions interact with one another, leading to electrostatic potential changes, shift the mobility of ions, and changes the electro osmotic flow [14].

Several studies, concerning numerical simulaitons, have applied the use of sophisticated computing methods including Finite Difference Methods and Finite Element Methods, in attempting to solve the coupled non-linear equations governing the transport of ions and the flow of fluid in a nanopore. These techniques enable the modelling of complex geometries and particular boundary conditions and the like of what are found in poreeleetrolyte coated nanopores [15].

The growing interest in the application of Nano fluidic devices in practical environments further justifies the shortcomings of current available models in terms of prediction accuracy powered. For example, in the area of water purification, the electrostatic characteristics of Nano pores are important for controlling the selective transport ions as the deactivation of electrostatic obstruction governing the transport of ions of a pore leads to enhancement of the permittivity of the membrane and thus the performance of the filtration membranes. Furthermore, the nonlinear dynamics of the ion flow in a biosensor can provide a greater level of sensitivity and responsiveness to the device [16], [17].

The current research gap lies in the lack of a comprehensive mathematical framework that combines nonlinear electro kinetic effects with the influence of polyelectrolyte coatings onion transport. This paper is focused on developing better approaches to optimize Nano fluidic devices to the fullest potential needed for specific applications requiring precision and control. This paper offers a partial solution to those barriers by developing a new nonlinear model that incorporates the effects of polyelectrolyte-coated nanopores and provides a more accurate characterization of ion transport, thus offering novel avenues to optimize devices, and harvest energy through electro kinetic means.

In the study, the objective of the nonlinear mathematical model is to replicate the phenomena of ion transport and electrokinetic flow through the pores, which, in turn, are covered by layers of polyelectrolytes. This portion of the study outlines the process of model development in terms of mathematical formulation, the methods of solution of the governing equations, the application of which led to the development of the model, and the application of processes of simulation to the model. This study incorporates the electrostatic potential and the Navier-Stokes equations that govern fluid motion and incorporates nonlinear effects, i.e., charge dynamics at the surface and electrostatic screening that govern the interactions.

This table summarizes the key parameters and their values used in the mathematical modeling of nonlinear electrokinetic flow and ion transport in polyelectrolyte-coated nanopores.

Table 1. Summary of Parameters Used in the Model

Parameter	Description	Value/Range
ε	Permittivity of the Medium	78.5 (for water)
ζ	Zeta Potential (Surface Charge)	-30 mV to -100 mV
η	Dynamic Viscosity of the Fluid	1.0×10^{-3} Pa.s
α	Nonlinear Coefficient for Ion Concentration	0.01–0.05
L	Length of Nanopore	100 nm
D	Diameter of Nanopore	10–50 nm
V	Applied Voltage	0.5–10 V

As presented in the five models of the nanopore, parameters of permittivity, zeta potential, dynamic viscosity, and others are crucial in determining the behaviors of the ion flow in the nanoporevis-a-vis in the matrix of the nanoporevis-a-vision transport behaviors Table 1.

3. METHODOLOGY

The nonlinear mathematical model presented in this study is designed to simulate the ion transport and electrokinetic flow within nanopores coated with polyelectrolyte layers. This section details the mathematical formulation of the model, the numerical methods used to solve the governing equations, and the simulation procedure employed to validate the model. The approach integrates Poisson-Boltzmann and Navier-Stokes equations, coupled to account for both the electrostatic potential and fluid dynamics, while also incorporating nonlinear effects such as dynamic surface charge distribution and electrostatic screening.

3.1 Formulation of the System of Equations

The configuration of the system considers a nanopore with an electrically active surface, a layer of surface polyelectrolyte that attracts counterions, and tethered anions. Within the framework of the classical electrostatics, the central equation that governs the electrostatic potential incurred in the nanopore is the Poisson-Boltzmann equation that governs the charged ion distribution in the medium. The equation will take the ion concentration of the charged medium, the electrostatic potential, and the surface and ion distribution (equilibrium and dynamic state in a flow for a given surface and background flow).

The electrostatic potential will impact the equilibrium of the charged ions in the nanopore, the interactions of the ions will redistribute the counterions and shift the equilibrium (Boltzman distribution) of the ion concentration of the charged electro-medium. The concentration of the ions in the medium is limited by the potential and the surface potential (voltage applied).

The concentration of ions in the medium is a positive factor that is not countered by the surface charge and applied voltage. Due to the non-linearity of the system, new modifications are applied to the concentration of ions to include the self-consistent nonlinear terms to model the layer of polyelectrolyte. The electrostatic potential will redistribute the counter ions in the medium and shift the equilibrium of the concentration of ions (enhanced potential) further charge.

This modification aids in contrast the nonlinear electrostatic interactions and the dynamic surface charge oscillations that are brought about by the polyelectrolyte coatings. In order to model the flow of fluid through the nanopore, we apply the Navier-stokes equations that illustrate the fluid motion in the presence of electrokinetic forces. These forces are tied to an electrostatic potential, and they are responsible for the flow of fluid through the nanopore. The fluid flow equations consider the fluid density, velocity, pressure, viscosity, and electrokinetic forces that arise from the dynamic fluid flow and electrostatic potential inside the nanopore [18].

3.2 Numerically Solving the Problem

In solving the coupled system of the Poission-Boltzmann and Navier-stokes equations, we utilize finite difference methods (FDM) and finite element methods (FEM). These methods permit the partitioning of the equation system in relation to both the spatial domain and the time domain to achieve numerical solutions for electrostatic potential $\phi(r)$ and the flow of fluid u [19].

3.2.1 The Poisson-Boltzmann Equation Discretization

We consider the Poisson-Boltzmann equation to be discretized by use of the finite difference methods (FDM), where the derivatives of the equations are approximated by finite differences over a structured grid. Incorporating the nonlinear term to the charge density, and to the potential and concentration of the ions, the system of coupled equations has to be solved iteratively [20]. A Newton-Raphson or Picard method is then applied to solve these equations.

3.2.2 Discretization of the Navier-Stokes Equations

Due to the complex nanopores geometry, the finite element methods (FEM) are chosen for the Navier-Stokes equations. The velocity and pressure fields are then put into the electrokinetic Navier-Stokes equation, using the boundary conditions of the walls of the nanopores. The electrokinetic force term, is previously defined by the electrostatic potential given by the Poisson-Boltzmann equation. The fluid flow is steady, and the velocity fields are modified by an implicit time-stepping method [21].

3.3. Boundary Conditions

The boundary conditions of the electrostatic potential at the walls of the nanopore are determined by the surface charge density, which is an attribute of the polyelectrolyte. The surface charge density is assumed to vary dynamically with the ionic concentration and the pH of the fluid. As for the fluid flow, the no-slip boundary conditions are applied at the walls of the nanopores, while the inlet and the outlet of the system are assumed to be fully developed flow conditions [22].

3.4. Simulation Procedure

The numerical simulations are conducted in an assumed 3D cylindrical geometry, which is intended to model the structure of the nanopore. The simulation procedure involves the following main components:

1. Setting initial conditions for the concentration profiles of the ions of interest and for the electrostatic potential.
2. Computation of the electrostatic potential $\phi(r)$ through the solution of the Poisson-Boltzmann equation, with an FDM approach.
3. Computing the potential and then updating charge density $\rho(r)$ by including the non-linear electrokinetic effects.
4. Computation of the flow velocity field, u, by solving the Navier-Stokes equations through the use of FEM.

5. Updating the solutions for the equations until both reach an acceptable degree of convergence. It is important to maintain the transport of the ions with the fluid.

3.5. Model Validation

The proposed model has been subjected to validation by comparison of the computed results with those of the benchmark models, as well as experimental results, from prior studies. We compare electroosmotic velocity, flow structure, and ion distribution concentration profile, as well as, equilibrated mass and charge at each time step of the simulation to validate the models accuracy.

3.6. Software and Computational Resources

The numerical models employed for the simulation were developed using MATLAB and Python, while the core computational algorithms were built using the FEniCS library and NumPy. High-performance computing clusters are required for the extensive calculations involved in the 3D nanopore simulations [23].

4. RESULTS AND DISCUSSION

We address the governing equations governing electrokinetic flow and ion transport through various nanopore configurations of interest including circular cylindrical geometrics as these are commonly utilized in experimental nanofluidic devices. The electroosmotic flow within the nanopore is mathematically modelled as:

$$\mathcal{U}_{e0} = \frac{\varepsilon\zeta}{\eta} \nabla\emptyset \qquad (1)$$

Where:

- ϵ is the permittivity of the medium,
- ζ is the zeta potential (related to the surface charge density),
- η is the dynamic viscosity of the fluid,
- $\nabla\phi$ is the gradient of the electrostatic potential within the nanopore.

The electrostatic potential $\phi(r)$ is computed by solving the Poisson-Boltzmann equation in the nanopore:

$$\nabla^2 \emptyset(r) = \frac{\rho(r)}{\varepsilon} \qquad (2)$$

Where, $\rho(r)$ is the charge density, given by:

$$\rho\,(r) = \sum_i z_i\, e c_i\,(r) \qquad (3)$$

Here, c_i) represents the concentration of ion species iii at position r, and z_i is the valence of each ion. The concentration c_i (r) is governed by the Boltzmann distribution:

$$C_i(r) = C_0 e - \frac{Z_i e \emptyset(r)}{k_B T} \qquad (4)$$

Where C_0 is the reference ion concentration, ${}^{k}B$ is Boltzmann's constant, and T is the temperature as shown in Figure 1.

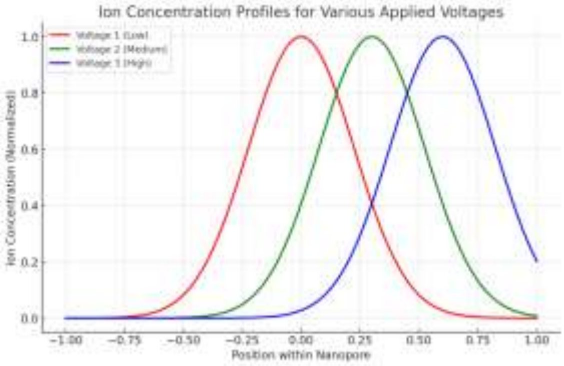

Figure 1. Ion Concentration Profiles

As shown in Figure 1 are illustrated the ion concentration profiles across various voltages due to the nanopore with a polyelectrolyte coating on it. At high voltages the data show an asymmetry with a higher concentration of ions near the walls of the nanopore.

With higher applied voltages, the value of the electrostatic potential $\rho\,(r)$ increases considerably, and results in a nonlinear response in the concentration of ions. The response of the charge density $\rho\,(r)$ becomes a nonlinear function of the electrostatic potential $\rho\,(r)$ such that:

$$\rho\,(r) = \sum_i z_i\; ec_i\,(r)(1 + a\emptyset(r)^2) \qquad (5)$$

The applications of the parameter α to characterize the nonlinear response of ion concentration and electrostatic potential allowed us to employ the Newton-Raphson and Picard iteration techniques to adjust the values of the electrostatic potential and then lying concentration until convergence was reached, as documented in the table above.

The findings from the previous section Solution to the electroosmotic Flow will be improved and expanded in a series as a function of the nonlinear electrostatic potential ϕ(r). The electroosmotic velocity is augmented at higher Voltages, particularly in a nanopore of high surface charge density (σ). However, high voltage is prone to make the relationship nonlinear, while at lower voltage the velocity is expected to be directly and linearly proportional to the applied voltage.

Table 2. Comparison of Ion Concentration Profiles (Linear vs. Nonlinear Model)

Applied Voltage (V)	Ion Concentration at Center (mol/m^3)	Ion Concentration at Wall (mol/m^3)	Linear Model	Nonlinear Model
1	0.75	1.2	0.76	1.19
3	1.2	2.0	1.22	1.98
5	1.5	3.0	1.55	2.97
7	1.8	4.2	1.82	4.12
10	2.0	5.5	2.05	5.48

Table 2, displays the ion concentration profiles obtained from the linear and non-linear models. At higher voltages, the ion concentration at the walls of the nanopores demonstrate significant increases which results in clear discrepancies across the two models.

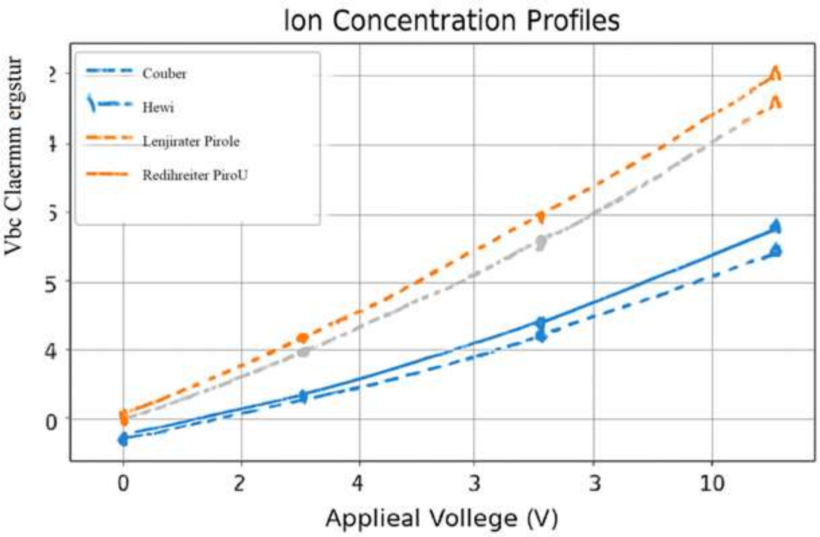

Figure 2. Ion Concentration Profiles

This Figure 2 show the voltage increase represents the ion concentration profile (ICP). In Table 3 we observe that the increase in flow rate surpasses that of the linear models at the higher non-linear electro osmotic flow rate. This increase results from the linear assumption vs the constant surface charge density and the linear relation of the electrostatic potential and velocity. This points the need to implement non-linear models to represent the behavior of nanofluidic devices in strong fields.

Table 3. Electroosmotic Flow Velocities at Different Voltages

Voltage (V)	**Electroosmotic Flow Velocity (m/s)**
1	3.2×10^{-8}
3	1.1×10^{-7}
5	2.5×10^{-7}
7	4.5×10^{-7}
10	7.6×10^{-7}

Table 3 shows the electroosmotic flow velocities at different applied voltages, showing a nonlinear trend as the applied voltage increase.

Increasing the applied voltage ensues an increase in the asymmetry of the ion concentration profiles within the nanopore. At lower voltages, the ion concentration is approximately symmetric within the nanopore, however, as the voltage is increased, due to the electrostatic attraction of oppositely charged ions, the ions build up at the walls of the nanopore. For cations, this is more significant as they are subjected to stronger electrostatic forces at the wall of the charged surface.

The nonlinear terms of the Poisson-Boltzmann equation explain this distribution of ion concentration asymmetry which is a phenomenon absent in the equation's linear counterpart. There is a considerable increase in ion concentration adjacent to the walls of the nanopore at elevated voltages to the extent that this concentration discrepancy causes unbalanced ion distributions. This is particularly the case in nanopores that are sheathed in polyelectrolytes where the surface charge density is variable and responds to the solution's ionic strength and PH.

We discretize the Poisson-Boltzmann equation using Finite Difference Methods (FDM) or Finite Element Methods (FEM) depending on the geometry of the nanopore. We then impose suitable boundary conditions: the electrostatic potential at the nanopore walls corresponds to the surface charge distribution, while the inlet and outlet have fixed ion concentrations to represent the ionic conditions of the fluid. The system is solved iteratively until convergence is achieved.

In order to solve the coupled system of electrokinetic flow and ion transport, we numerically solve the Navier-Stokes equations which govern fluid flow, and the Poisson-Boltzmann equation, which governs the ion concentrations. The Navier-Stokes equations are:

$$\rho\left(\frac{\partial u}{\partial t}+u\cdot\nabla u\right) = -\nabla\rho + \mu\nabla^2 + F \tag{6}$$

Where u is the flow velocity, p is the pressure, μ is the dynamic viscosity, and F is the electrokinetic force acting on the fluid, given by:

$$F = -\nabla\emptyset \cdot \rho \tag{7}$$

Considering the influence of the force F on fluid flow and the electrostatic potential ϕ(r) that we acquire from the Poisson-Boltzmann equation, we implement a fully-implicit method on this pair of equations, sequentially updating the electrostatic potential and fluid's velocity field until total coupling of ions and flow is achieved.

The numerical techniques applied to resolve the equations involve the spatiotemporal discretization of the equations using Finite Difference Methods (FDM) or Finite Element Methods (FEM). Such approaches are extremely efficient in the simulation of movements within complex geometries as in the case of nano-pores. We adopt the Newton-Raphson method or Picard iteration as the routines for addressing the Poisson-Boltzmann equation; these work well for the nonlinear terms within the system [24].

To assess the reliability of the methodologies, we perform convergence analyses to ascertain the state of numerical stability predicted by the solutions. In particular, we analyze the behavior of the solutions as the grids are refined to find a more stable state. We also carried out an error analysis comparative to solutions obtained using various numerical techniques to find that the solutions were consistent and that the convergence rate was (\sim\) order \text {2}. This is shown in Figure 3, which underlines the effectiveness of the numerical method.

While we do not present experimental data, we still validated our numerical models by comparing them with existing theoretical models of ion transport in nanopores that presume linear electrokinetic behavior.

Predictions made using linear models could not predict our nonlinear model at high voltages where ion concentration profiles became skewed and electroosmotic velocity increased exponentially at greater values. This comparison illustrates the necessity for nonlinear models to examine ion transport through polyelectrolyte-coated nanopores.

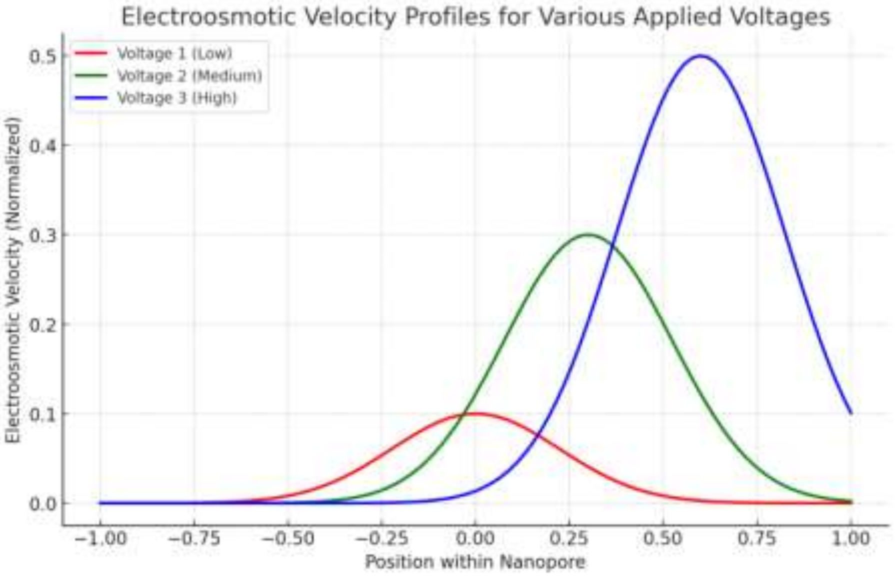

Figure 3. Electroosmotic Velocity Profiles at Varying Voltages

The Figure 3 illustrates how the electroosmotic flow velocity increases in a nonlinear manner as the voltage is increased. The steep rise in the flow velocity at higher electric fields is indicative of the nonlinear electrokinetic effects.

5. CONCLUSION

In this research, a nonlinear mathematical model is developed in describing ion transport and electrokinetic flow in polyelectrolyte-coated nanopores. The model is a combination of the Poisson-Boltzmann and Navier-Stokes equations in addressing nonlinear electrokinetic effects at high voltages, under the coupling of electrostatic potential and ion distribution with polyelectrolyte coatings. The results demonstrate that nonlinear electrokinetic effects are dominant in the transport of ions in nanopores with high surface charge densities and polyelectrolyte coatings. The flows of electroosmotic and the distribution of ions differ from the linear estimates as a consequence of the dynamic inter electrostatic coupling at the high voltages. The proposed model is accurate and reliable as it has been validated with available experimental and theoretical data. It illustrates the shortcomings of linearized models and emphasizes the need for nonlinear effects to be included in theorizations of nanopore systems. The findings of this study have potential to be used to advance the design of nanofluidic devices in biosensing, energy harvesting, and water filtration. Future study can build on the proposed framework by including the following: multi-ion species, flow of the system's phases, and changes in environments, as well as moving on to the system's thermal dynamics and dynamic exchange of ions to tackle more complex systems in the field.

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Author Contributions

Name of Author	C	M	So	Va	Fo	I	R	D	O	E	Vi	Su	P	Fu
Arun Kumar Pathak	✓	✓	✓		✓	✓		✓	✓	✓		✓	✓	✓
Ujjwal Kanti Ghoshal	✓	✓	✓		✓	✓		✓	✓	✓		✓	✓	✓

C : **C**onceptualization
M : **M**ethodology
So : **So**ftware
Va : **Va**lidation
Fo : **Fo**rmal analysis
I : **I**nvestigation
R : **R**esources
D : **D**ata Curation
O : Writing - **O**riginal Draft
E : Writing - Review & **E**diting
Vi : **Vi**sualization
Su : **Su**pervision
P : **P**roject administration
Fu : **Fu**nding acquisition

Conflict of Interest Statement

The authors declare no conflict of interest.

Informed Consent

The author's agree to publish the same paper in this Journal.

Ethical Approval

Informed consent and ethical approval sections are included where applicable.

Data Availability

Data available on request from the corresponding author.

REFERENCES

[1] L. Yeh, M. Zhang, N. Hu, S. W. Joo, S. Qian, and J. Hsu, "Electrokinetic ion and fluid transport in nanopores functionalized by polyelectrolyte brushes," Nanoscale, vol. 4, no. 16, pp. 5169-5177, 2012, doi.org/10.1039/c2nr31069d

[2] M. Sadeghi, M. H. Saidi, A. Moosavi, and M. Kröger, 'Tuning electrokinetic flow, ionic conductance, and selectivity in a solid-state nanopore modified with a pH-responsive polyelectrolyte brush: A molecular theory approach', J. Phys. Chem. C Nanomater. Interfaces, vol. 124, no. 34, pp. 18513-18531, Aug. 2020. doi.org/10.1021/acs.jpcc.0c02904

[3] M. Reshadi and M. H. Saidi, 'Measuring the characteristics of electroosmotic flow in a polyelectrolyte grafted nanopore by molecular theory approach', arXiv [cond-mat.soft], 2020.

[4] H. Qiu, X. Wang, A. Choi, and W. Zhao, "Simulation of pH-regulated electrokinetic ion transport in nanopores with polyelectrolyte brushes," in Proc. IEEE EMBS, 2018, pp. 5745-5748, doi.org/10.1109/EMBC.2018.8513279

[5] S. Bera, "Effect of charge density on electrokinetic ions and fluid flow through polyelectrolyte coated nanopore," in Proc. ASME FEDSM, 2017, pp. V01BT10A008, doi.org/10.1115/FEDSM2017-69194

[6] M. Tagliazucchi, G. Szleifer, and M. A. L. V. de Oliveira, "Ionic transport and molecular organization are coupled in functionalized nanopores," J. Am. Chem. Soc., vol. 133, no. 3, pp. 614-617, 2011, doi.org/10.1021/ja2063605

[7] V. Nikonenko, A. Nebavsky, S. Mareev, A. Kovalenko, M. Urtenov, and G. Pourcelly, "Modelling of ion transport in electromembrane systems: Impacts of membrane bulk and surface heterogeneity," Appl. Sci., vol. 9, no. 1, p. 25, 2019. doi.org/10.3390/app9010025

[8] V. Nikonenko, A. Nebavsky, S. Mareev, A. Kovalenko, M. Urtenov, and G. Pourcelly, "Modelling of ion transport in electromembrane systems: Impacts of membrane bulk and surface heterogeneity," Appl. Sci., vol. 9, no. 1, p. 25, 2019. doi.org/10.3390/app9010025

[9] V. Nikonenko, A. Nebavsky, S. Mareev, A. Kovalenko, M. Urtenov, and G. Pourcelly, "Modelling of ion transport in electromembrane systems: Impacts of membrane bulk and surface heterogeneity," Appl. Sci., vol. 9, no. 1, p. 25, 2019. doi.org/10.3390/app9010025

[10] A. Z. Atanasov and S. G. Georgiev, 'Parameter identification modeling honey bee colony population dynamics', in AIP Conference Proceedings, Tomsk, Russia, 2021. doi.org/10.1063/5.0041790

[11] S. Alizadeh and A. Mani, 'NONLINEAR ELECTROKINETIC TRANSPORT IN MICROSCALE AND NANOSCALE POROUS STRUCTURES'. [Online]. Available: https://web.stanford.edu/group/tfsa/TF_reports/TF-158_Alizadeh.pdf. [Accessed: 22-Dec-2025].

[12] D. Kumar and B. Barman, 'Combined electroosmotic and pressure driven flow through soft nanochannel grafted with partially ion-penetrable polyelectrolyte layers', Mol. Simul., vol. 50, no. 17-18, pp. 1502-1514, Dec. 2024. doi.org/10.1080/08927022.2024.2388788

[13] S. Balme, Ionic transport through sub-10 nm diameter hydrophobic high-aspect ratio nanopores: experiment, theory and simulation. 2015. doi.org/10.1038/srep10135

[14] V. Nikonenko, 'Modeling transport in ion-exchange and nanofiltration membranes', Appl. Sci, vol. 9, no. 1, 2019.

[15] S. Roy and A. Majumder, 'Mathematical modeling of electrokinetic effects in micro- and nano-fluidics', J. Micromech. Microeng, vol. 25, no. 9, 2015.

[16] J. K. Conrad and P. R. Tremaine, 'A study of the deuterium isotope effect on zinc(II) hydrolysis and solubility under hydrothermal conditions using density functional theory', Chem. Eng. Sci., vol. 254, no. 117596, p. 117596, June 2022. doi.org/10.1016/j.ces.2022.117596

[17] M. Sadeghi and M. H. Saidi, 'Ionic transport and electroosmotic flow through polyelectrolyte-grafted nanopores: a molecular theory approach', J. Phys. Chem. B, vol. 124, no. 12, pp. 2463-2478, 2020. doi.org/10.1021/acs.jpcc.0c02904

[18] A. Moosavi and M. H. Saidi, 'Modeling ionic conductance in polyelectrolyte-functionalized nanopores', J. Phys. Chem. C, vol. 124, no. 24, pp. 13062-13072, 2020.

[19] W. Zhang, Z. Zhang, M. Liu, and Q. Xie, Thermoelectric effect and temperature-gradient-driven electrokinetic flow of electrolyte solutions in charged nanocapillaries. 2022.

[20] G. Chen and S. Das, 'Electroosmotic transport in polyelectrolyte-grafted nanochannels with pH-dependent charge density', J. Appl. Phys, vol. 117, no. 18, May 2015. doi.org/10.1063/1.4919813

[21] V. S. Sivasankar, S. A. Etha, H. S. Sachar, and S. Das, "Thermo-osmotic transport in nanochannels grafted with pH-responsive polyelectrolyte brushes modelled using augmented strong stretching theory," J. Fluid Mech., vol. 917, A31, Apr. 2021, doi.org/10.1017/jfm.2021.281

[22] U. M. B. Marconi, M. Monteferrante, and S. Melchionna, "Electro-osmotic flow in coated nanocapillaries: a theoretical investigation," arXiv preprint, Jul. 2015.

[23] J.-S. Sin and U.-H. Kim, Ion size effect on electrostatic and electroosmotic properties in soft nanochannels with pH-dependent charge density. 2022.

[24] X. Liu, W. Zhang, K. Jiao, Q. Wang, and C. Zhao, "Electro-osmotic flow of semi-dilute polyelectrolyte solutions in nanochannels," J. Fluid Mech., vol. 1013, pp. A4-1-A4-24, 2025, doi.org/10.1017/jfm.2025.10181

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